UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
WASHINGTON, D.C. 20460

OFFICE OF
PREVENTION, PESTICIDES, AND
TOXIC SUBSTANCES

MEMORANDUM

DATE: November 10, 2009

SUBJECT: Revision of Input Parameter Guidance

FROM: Donald Brady, Division Director
Environmental Fate and Effects Division (7507P)
Office of Pesticide Programs

D Brady 11/10/09

TO: Environmental Fate and Effects Division (7507P)
Office of Pesticide Programs

This memorandum announces the release of Version 2.1 of the existing Input Parameter Guidance for a suite of models used in EFED, including SCI-GROW, GENEEC, FIRST, PRZM, and EXAMS. General updates as well as model-specific updates were made to the guidance. General updates include:

- Parameter descriptions were reformatted, updated to better resemble how they appear in the models, and re-ordered to reflect their order in the models.
- Guidance on how to calculate the 90th percentile of the mean was moved to an appendix.
- Soil-water partition coefficients were harmonized across the surface water models;
- Incorporation depths for different application methods were added.
- Output file-related parameters not addressed in the previous guidance were addressed;
- Additional editorial corrections and clarifications were made.

In general, any aquatic modeling that begins on or after the week of November 16, 2009 should be conducted with Version 2.1 of the Input Parameter Guidance (dated October 22, 2009). Aquatic exposure modeling begun prior to November 16, 2009 may be completed using Version II of the Input Parameter Guidance (dated February 28, 2002).

Attachments:

1) Input Parameter Guidance (Version 2.1; October 22, 2009).

Guidance for Selecting Input Parameters in Modeling the Environmental Fate and Transport of Pesticides

Version 2.1

October 22, 2009

U.S. Environmental Protection Agency
Office of Pesticide Programs
Environmental Fate and Effects Division

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1.0 Introduction

EPA's Office of Pesticide Programs (OPP) has developed this guidance document to help model users select and prepare the appropriate input values for OPP's aquatic exposure models. Using this guidance document should improve the consistency in modeling the fate of pesticides in the environment and ultimately the overall quality of OPP's aquatic risk assessments. The primary sources of input fate parameters that are used in these models include pesticide product chemistry and labeling information as well as sorption coefficients, half-lives, and rate constants from acceptable or supplemental environmental fate studies conducted or sponsored by pesticide manufacturers.

2.0 Summary Guidance Tables for Model Input Parameters

The guidance tables listed below contain the parameters, input values, sources of data, and additional explanatory information (notes) for the following aquatic exposure models: SCI-GROW, GENEEC, FIRST, PRZM, and EXAMS. More specific information about these aquatic models can be found at the following web site: http://www.epa.gov/oppefed1/models/water/index.htm. For specific cases, in which deviation from the guidance is appropriate, the model user should document the rationale for each deviation. If additional guidance is necessary, OPP model users should consult with the Environmental Fate and Effects Division (EFED) Water Quality Technology Team (WQTT).

2.1 SCI-GROW

Table 2.1 Input Parameters for SCI-GROW (Version 2.3, July 29, 2003)

Parameter (units)	Input Value	Data Source	Notes
Output file	Select any file name and extension for the output file.		SCI-GROW will assign the extension ".txt" to the file name only if the "output file" button is pressed.
Chemical name	(User's choice)		
Application rate (lbs a.i./acre)	Use the maximum single application rate allowed on the label for the modeled use.	Product labels	
Number of applications	Use the maximum number of applications allowed on the label for the modeled use.	Product labels	
K_{OC} (mL/g_{oc})	If the partition coefficients normalized for organic carbon content (K_{OC} or K_{FOC}) show greater than a three-fold variation, use the lowest value. If not, then use the median value.	Adsorption/desorption data (OPPTS Guideline 835.1230)	SCI-GROW was developed using K_{OC} values ranging from 32-180 mL g_{OC}^{-1} and half-lives from 13-1000 days. Extrapolation beyond these values will increase the uncertainty of the ground water concentration. (The model will not use K_{OC} values >9995 mL g_{OC}^{-1}.)
Soil metabolism half-life (days)	If three or less aerobic soil metabolism half-life values are available, use the mean value. If there are four or more half-lives available, use the median value. If there is more than a five-fold difference, make note of the range.	Aerobic soil metabolism data (OPPTS Guideline 835.4100)	

2.2 GENEEC

Table 2.2 Input Parameters for GENEEC (Version 2.0, August 1, 2001)

Parameter (units)	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Run number	Select any number to associate with the results of this run in the output file.	Not applicable	
Output file name	Select up to 8 characters for the output file name followed by any 3-character extension.	Not applicable	GENEEC will not assign an extension to the file name.
Chemical name	Select any input with which to identify your chemical.	Product labels	
Crop name	Select any input with which to identify the modeled use.	Product labels	
Application rate (pounds a.i. per acre)	Use the maximum application rate specified on the label for the modeled use.	Product labels	When this information is not available on the label, determine a reasonable conservative estimate.
Number of applications	Use the maximum number of applications specified on the label for the modeled use.	Product labels	
Interval between applications (days)	Use the minimum application interval specified on the label for the modeled use.	Product labels	
Partition Coefficient K_d (mL g^{-1}) or K_{OC} (mL g_{OC}^{-1})	If binding is correlated with organic carbon content, enter zero (0) for K_d and then enter the mean K_{OC}. Otherwise, enter the mean K_d.	Adsorption/ desorption data (OPPTS Guideline 835.1230)	Binding is correlated with organic carbon content if the coefficient of variation (*i.e.*, the standard deviation divided by the mean) for K_{OC} values is less than that for K_d values.

Parameter (units)	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Soil aerobic metabolic half-life (days)	If multiple aerobic soil metabolism half-life values are available, enter the 90th percentile confidence bound on the mean half-life value (see Equation 1 in **Appendix A** for instructions). If a single aerobic soil metabolism half-life value is available, enter 3x the half-life value (see Equation 2 in **Appendix A**). If no aerobic soil metabolism data are available, assume that the compound is stable to biodegradation under these conditions, *i.e.*, enter zero (0).	Aerobic soil metabolism data (OPPTS Guideline 835.4100)	
Wetted in?	No	Product labels	In practice, "wetting in" is used to reduce the amount of pesticide available for runoff. With GENEEC, though, selecting the "wetting in" option changes the timing of the storm from two days after last application to immediately after the last application. The result is that pesticide concentrations may be greater, not less, especially for pesticides with a short half-life.
Method of application	Select (A) aerial, (B) ground, (C) air-blast spray, or (D) granular application.	Product labels	Lettered inputs are not case specific (*e.g.*, (A) or (a)).
⇨ **Droplet size distribution <under (A)>**	Select (A) very fine to fine, (B) fine to medium, (C) medium to coarse, or (D) coarse to very coarse.	Product labels	Select (B) fine to medium droplet size distribution if the label does not specify a coarser spray quality.
⇨ **Nozzle height <under (B)>**	For ground applications, select (A) low or (B) high boom ground sprayer.	Product labels	Select the high boom height as a default when it is not prohibited on the label.

Parameter (units)	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
⇨**Spray quality <under (B)>**	For ground applications, select (A) fine or (B) medium-course droplet size distribution.	Product labels	Select the fine droplet size distribution when it is not prohibited on the label.
⇨**Air-blast type <under (C)>**	Select (A) orchards and dormant vineyards or (B) foliated vineyards.	Product labels	
⇨**Width of no-spray zone (feet) <under (A), (B), or (C)>**	If specified on the label, enter the width of the no-spray (buffer) zone between the treated field and the water body.	Product labels	Select zero (0) ft if the label does not specify a buffer width.
⇨**Depth of incorporation (inches) <under (B) or (D)>**	Enter a depth of soil incorporation based on the information specified on the label. If the pesticide is not incorporated, use zero (0).	Product labels	Suggested incorporation depths include: Application Method — Depth (in) Broadcast — 0.0 Disked in — 4.0 Chisel plowed — 6.0 Surface banded — 0.0 Banded, incorporated — 1.2 T-banded — 1.5 In furrow — 2.0 Aerial or air-blast spray — 0.0 Ground spray — Depends on method
Solubility in water (ppm)	Use the maximum available value at 20-25°C.	Water solubility data (OPPTS Guideline 830.7840, 830.7860)	

Parameter (units)	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Aerobic aquatic metabolism half-life (days)	If multiple aerobic aquatic metabolism half-life values are available, enter the 90th percentile confidence bound on the mean half-life value for the total system (water plus sediment) (see Equation 1 in **Appendix A** for instructions). If a single aerobic aquatic metabolism half-life value is available, enter 3x the half-life value (see Equation 2 in **Appendix A**). If no aerobic aquatic metabolism data are available and the pesticide shows insignificant hydrolysis, use 2x the aerobic soil metabolism half-life input value. If no aerobic aquatic metabolism data are available and the pesticide shows significant hydrolysis, enter zero (0).	Aerobic aquatic metabolism data (OPPTS Guideline 835.4300)	This input parameter implies degradation by both metabolism and hydrolysis. If a positive value is entered, the model will NOT prompt for an independent hydrolysis rate (see hydrolysis section). Example for the case when no aerobic aquatic data are available and the pesticide is hydrolytically stable: For a single aerobic soil metabolism half-life of 30 days, the aerobic soil metabolism half-life input value is 90 days (30 days x 3); thus the estimated aerobic aquatic metabolism half-life input value is 180 days (90 days x 2).
⇨**Hydrolysis half-life (days)**	If zero (0) was entered for the aerobic aquatic metabolism half-life, enter the maximum hydrolysis half-life value at pH 7. If no hydrolysis data are available, enter zero (0) and assume the compound is stable.	Hydrolysis data (OPPTS Guideline 835.2120)	GENEEC prompts for the hydrolysis half-life only if a zero (0) is entered for the aerobic aquatic metabolism half-life.
Photolysis half-life (days)	Enter the maximum dark-control corrected environmental aqueous phototransformation half-life value. If no aqueous photolysis data are available or if there is no evidence of photolysis, enter zero (0).	Aqueous photolysis data (OPPTS Guideline 835.2240)	

2.3 FIRST

Table 2.3 Input Parameters for FIRST (Version 1.1.1, March 26, 2008)

Parameter (units)	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Run number	Select any number to associate with the results of this run in the output file.	Not applicable	
Output file name	Select up to 8 characters for the output file name followed by any 3-character extension.	Not applicable	FIRST will not assign an extension to the file name.
Chemical name	Select any input with which to identify your chemical.	Product labels	
Crop name	Select any input with which to identify the modeled use.	Product labels	
Application rate (pounds a.i. per acre)	Use the maximum application rate specified on the label for the modeled use.	Product labels	When this information is not available on the label, determine a reasonable conservative estimate.
Number of applications	Use the maximum number of applications specified on the label for the modeled use.	Product labels	
Interval between applications (days)	Use the minimum application interval specified on the label for the modeled use.	Product labels	
Percent cropped area (decimal)	Enter the maximum fraction of watershed planted in crops on which the pesticide may be applied.	PCA-specific guidance (values are suggested within the program and in the FIRST User's Manual)	
Partition coefficient K_d (mL g^{-1}) or K_{oc} (mL g_{oc}^{-1})	If binding is correlated with organic carbon content, enter zero (0) for K_d and then enter the mean K_{OC}. Otherwise, enter the mean K_d.	Adsorption/ desorption data (OPPTS Guideline 835.1230)	Binding is correlated with organic carbon content if the coefficient of variation (*i.e.*, the standard deviation divided by the mean) for K_{OC} values is less than that for K_d values.

Parameter (units)	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Aerobic soil metabolism half-life (days)	If multiple aerobic soil metabolism half-life values are available, enter the 90th percentile confidence bound on the mean half-life value (see Equation 1 in **Appendix A** for instructions). If a single aerobic soil metabolism half-life value is available, enter 3x the half-life value (see Equation 2 in **Appendix A**). If no aerobic soil metabolism data are available, assume that the compound is stable to biodegradation under these conditions, *i.e.*, enter zero (0).	Aerobic soil metabolism data (OPPTS Guideline 835.4100)	
Wetted in?	No	Product labels	In practice, "wetting in" is used to reduce the amount of pesticide available for runoff. With FIRST, though, selecting the "wetting in" option changes the timing of the storm from two days after last application to immediately after the last application. The result is that pesticide concentrations may be greater, not less, than wetting in especially for pesticides with a short half-life.
Method of application	Select (A) aerial, (B) ground, (C) air-blast spray, or (D) granular application.	Product labels	

Parameter (units)	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
⇨**Depth of incorporation (inches) <under (B) or (D)>**	Enter a depth of soil incorporation based on the information specified on the label. If the pesticide is not incorporated, use zero (0).	Product labels	Suggested incorporation depths include: Application Method — Depth (in) Broadcast — 0.0 Disked in — 4.0 Chisel plowed — 6.0 Surface banded — 0.0 Banded, incorporated — 1.2 T-banded — 1.5 In furrow — 2.0 Aerial or air-blast spray — 0.0 Ground spray — Depends on method
Solubility in water (ppm)	Use the maximum available value at 20-25°C.	Water solubility data (OPPTS Guideline 830.7840, 830.7860)	

Parameter (units)	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Aerobic aquatic metabolism half-life (days)	If multiple aerobic aquatic metabolism half-life values are available, enter the 90th percentile confidence bound on the mean half-life value for the total system (water plus sediment) (see Equation 1 in **Appendix A** for instructions). If a single aerobic aquatic metabolism half-life value is available, enter 3x the half-life value (see Equation 2 in **Appendix A**). If no aerobic aquatic metabolism data are available and the pesticide shows insignificant hydrolysis, use 2x the aerobic soil metabolism half-life input value. If no aerobic aquatic metabolism data are available and the pesticide shows significant hydrolysis, enter zero (0).	Aerobic aquatic metabolism data (OPPTS Guideline 835.4300)	This input parameter implies degradation by both metabolism and hydrolysis. If a positive value is entered, the model will NOT prompt for an independent hydrolysis rate (see hydrolysis section). Example for the case when no aerobic aquatic data are available and the pesticide is hydrolytically stable: For a single aerobic soil metabolism half-life of 30 days, the aerobic soil metabolism half-life input value is 90 days (30 days x 3); thus the estimated aerobic aquatic metabolism half-life input value is 180 days (90 days x 2).
⇨**Hydrolysis half-life (days)**	If zero (0) was entered for the aerobic aquatic metabolism half-life, enter the maximum hydrolysis half-life value at pH 7. If no hydrolysis data are available, enter zero (0) and assume the compound is stable.	Hydrolysis data (OPPTS Guideline 835.2120)	FIRST prompts for the hydrolysis half-life only if a zero (0) is entered for the aerobic aquatic metabolism half-life.
Photolysis half-life (days)	Enter the maximum dark-control corrected environmental aqueous phototransformation half-life value. If no aqueous photolysis data are available or if there is no evidence of photolysis, enter zero (0).	Aqueous photolysis data (OPPTS Guideline 835.2240)	

2.4 PRZM

The following guidance table is for running PRZM directly rather than through a graphical user interface (GUI) to estimate exposure in runoff. The main difference with using GUIs is that they typically require half-lives (in values of days) rather than rate constants (in values of day^{-1}) for metabolism parameters.

Table 2.4 Input Parameters for PRZM (Version 3.12.2, May 12, 2005)

Parameter (units)	PRZM Variable	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Application date(s) (day/mo/yr)	APD, APM, IAPYR	Use the maximum number of applications and minimum application interval for the modeled use.	Product labels or location-specific	The model user should consider location-specific cropping dates and relevant label-specific information. Other relevant information may be obtained from agricultural extension agents, crop experts (land-grant universities, grower groups), and BEAD.
Incorporation depth (cm)	DEPI	Use the information specified on the label for soil incorporation. If the pesticide is not incorporated, use zero (0).	Product labels	
Application rate (kg a.i. ha^{-1})	TAPP	Use the maximum application rate allowed per application for the modeled use.	Product labels	
Application efficiency (decimal)	APPEFF	Use 0.95 for aerial spray and 0.99 for ground spray and orchard air-blast.		
Spray drift fraction (decimal)	DRFT	For aquatic ecological exposure assessment, use 0.05 for aerial spray, 0.03 for orchard air-blast, or 0.01 for ground spray.		
		For drinking water assessment, use 0.16 for aerial spray, 0.064 for ground spray, or 0.063 for orchard air-blast.	Spray Drift Task Force data	Spray drift fractions for drinking water exposure modeling are based upon the Spray Drift Task Force studies. See http://www.epa.gov/oscpmont/sap/meetings/1998/index.htm#072998 (SAP meeting, July 29-30, 1998)

Parameter (units)	PRZM Variable	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Foliar extraction (cm^{-1})	FEXTRC	Enter 0.5 (default value) unless field data are available.		Note that this parameter is a rate constant (cm^{-1}), not a depth (cm) of 50% wash-off (WD_{50}).
Decay rate on foliage (day^{-1})	PLDKRT	If multiple foliar decay half-life values are available, enter the rate constant corresponding to the upper 90th percentile confidence bound on the mean half-life value (see Equations 1 and 3 in **Appendix A** for instructions). If a single foliar decay half-life value is available, enter the rate constant corresponding to 3x the half-life value (see Equations 2 and 3 in **Appendix A**). If no foliar decay data are available, assume that the compound does not decay on foliage, *i.e.*, enter zero (0).	Magnitude of the residue or greenhouse foliar decay data	Note that this parameter is a rate constant (day^{-1}), not a half-life (day).
Volatilization rate from foliage (day^{-1})	PLVKRT	Enter zero (0) unless field data are available.		Note that this parameter is a rate constant (day^{-1}), not a half-life (day).
Plant uptake factor (decimal)	UPTKF	Enter zero (0) unless field data are available.		

Parameter (units)	PRZM Variable	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Dissolved phase pesticide decay rate in surface horizon (day^{-1})	DWRATE (surface)	DWRATE = DSRATE If multiple aerobic soil metabolism half-life values are available, enter the rate constant corresponding to the 90th percentile confidence bound on the mean half-life value (see Equations 1 and 3 in **Appendix A** for instructions). If a single aerobic soil metabolism half-life value is available, enter the rate constant corresponding to 3x the half-life value (see Equations 2 and 3 in **Appendix A**). If no aerobic soil metabolism data are available, assume that the compound is stable to biodegradation under these conditions, *i.e.*, enter zero (0).	Aerobic soil metabolism data (OPPTS Guideline 835.4100)	Although EFED rarely receives horizon-specific studies, separate chemical-specific inputs can be created for each horizon. The surface horizon is the most critical horizon for modeling runoff in PRZM. Note that these parameters are rate constants (day^{-1}), not half-lives (day).
Adsorbed phase pesticide decay rate in surface horizon (day^{-1})	DSRATE (surface)			

Parameter (units)	PRZM Variable	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Dissolved phase pesticide decay rate in subsequent subsurface horizons (day^{-1})	DWRATE (subsurface horizons)	DWRATE = DSRATE If multiple relevant soil metabolism half-life values are available (see notes), enter the rate constant corresponding to the 90th percentile confidence bound on the mean half-life value (see Equations 1 and 3 in **Appendix A** for instructions).	Aerobic or anaerobic soil metabolism data (OPPTS Guideline 835.4100, 835.4200)	Pesticide degradation below 2 cm does not influence PRZM runoff concentrations, so parameterization of horizon degradation below 2 cm is rarely necessary (scenarios developed for the PRZM volatilization routines are an exception). Note that these parameters are rate constants (day^{-1}), not half-lives (day).
Adsorbed phase pesticide decay rate in subsequent subsurface horizons (day^{-1})	DSRATE (subsurface horizons)	If a single relevant soil metabolism half-life value is available (see notes), enter the rate constant corresponding to 3x the half-life value (see Equations 2 and 3 in **Appendix A**). If no relevant soil metabolism data are available, assume that the compound is stable to biodegradation under these conditions, *i.e.*, enter zero (0).		

Parameter (units)	PRZM Variable	Input Value [*Specific Parameter Guidance*]	Data Source	Notes

Pesticide partition or distribution coefficients for each horizon (cm^3 g^{-1})	KD	If binding is correlated with organic carbon content, use the mean K_{OC}:
		
		- Set K_ds in Record 37 to 0.0
		- Set KDFLAG = 1
		- Then modify Record 30:
		  - set PCMC = 4
		  - set SOL = mean K_{OC}
		
		If binding is not correlated with organic carbon content, use the mean K_d:
		
		- Set KDFLAG in Record 20 = 0 (the default value in the standard scenarios)
		- In Record 37, input individual K_ds for each layer
			Adsorption/ desorption data (OPPTS Guideline 835.1230)	Binding is correlated with organic carbon content if the coefficient of variation (*i.e.*, the standard deviation divided by the mean) for K_{OC} values is less than that for K_d values.
				
				Use of the mean Kd may not be appropriate for certain chemicals with binding not correlated with organic carbon content, such as those that are ionic at environmental pH values. In these cases, the model user should document the rationale for the selected model input values. Additional guidance may be sought at the EFED WQTT.

2.5 EXAMS

The following guidance table is for running EXAMS directly rather than through a graphical user interface (GUI). The main difference with using GUIs is that they typically require half-lives (in units of days) rather than rate constants (in units of $hour^{-1}$) for metabolism, hydrolysis, and photolysis parameters.

Table 2.5 Input Parameters for EXAMS (Version 2.98.4.6, April 25, 2005)

Parameter (units)	EXAMS Variable	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Henry's Law Constant ($atm\text{-}m^3/mole$)	HENRY (1)	Use the measured Henry's Law Constant from submitted product chemistry data. If a measured value is not available, calculate the value from HENRY = (VAPR/760)/(SOL/MWT), where VAPR is vapor pressure in torrs, MWT is the molecular weight in g mol^{-1}, and SOL is the solubility in water in mg L^{-1}.	Product chemistry data	

Parameter (units)	EXAMS Variable	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Bacterial biolysis in water column $(cfu/mL)^{-1}$ $hour^{-1}$	KBACW (*,*,1)	If multiple aerobic aquatic metabolism half-life values are available, enter the rate constant (in units of $hour^{-1}$) corresponding to the 90th percentile confidence bound on the mean half-life value for the total system (water plus sediment) (see Equations 1 and 3 in **Appendix A** for instructions). If a single aerobic aquatic metabolism half-life value is available, enter the rate constant (in units of $hour^{-1}$) corresponding to 3x the half-life value (see Equations 2 and 3 in **Appendix A**). If no aerobic aquatic metabolism data are available and the pesticide shows insignificant hydrolysis, use (1/48)x the PRZM aerobic soil metabolism rate constant input value (DWRATE), *i.e.*, use the rate constant corresponding to 2x the half-life corresponding to the PRZM aerobic soil metabolism rate constant input value and convert units from day^{-1} to $hour^{-1}$. If no aerobic aquatic metabolism data are available and the pesticide shows significant hydrolysis, assume that the compound is stable to aerobic aquatic metabolism, *i.e.*, enter zero (0).	Aerobic aquatic metabolism data (OPPTS Guideline 835.4300)	When both aquatic metabolism and hydrolysis rate data are included, the metabolism rate needs to be corrected for the hydrolysis rate at the pH of the aquatic metabolism study. EXAMS calls for second-order rate constants normalized by bacterial "colony forming units". Colony forming units are fixed at 1 cfu ml^{-1}. Note that this parameter is a rate constant ($hour^{-1}$), not a half-life (hour). Also note that EXAMS rate constants are in units of $hour^{-1}$, not day^{-1}, as in PRZM.

Parameter (units)	EXAMS Variable	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Bacterial biolysis in benthic sediment (cfu/mL)$^{-1}$ hour^{-1}	KBACS (*,*,1)	If multiple anaerobic aquatic metabolism half-life values are available, enter the rate constant (in units of hour^{-1}) corresponding to the 90th percentile confidence bound on the mean half-life value for the total system (water plus sediment) (see Equations 1 and 3 in **Appendix A** for instructions). If a single anaerobic aquatic metabolism half-life value is available, enter the rate constant (in units of hour^{-1}) corresponding to 3x the half-life value (see Equations 2 and 3 in **Appendix A**). If no anaerobic aquatic metabolism data are available and the pesticide shows insignificant hydrolysis, use (1/48)x the PRZM anaerobic soil metabolism rate constant input value (DWRATE), *i.e.*, use the rate constant corresponding to 2x the half-life corresponding to the PRZM anaerobic soil metabolism rate constant input value and convert units from day^{-1} to hour^{-1}. If no anaerobic aquatic metabolism data are available and the pesticide shows significant hydrolysis, assume that the compound is stable to anaerobic aquatic metabolism, *i.e.*, enter zero (0).	Anaerobic aquatic metabolism data (OPPTS Guideline 835.4400)	When both aquatic metabolism and hydrolysis rate data are included, the metabolism rate needs to be corrected for the hydrolysis rate at the pH of the aquatic metabolism study. The model calls for second-order rate constants normalized by bacterial "colony forming units". Colony forming units are fixed at 1 cfu ml^{-1}. Note that this parameter is a rate constant (hour^{-1}), not a half-life (hour). Also note that EXAMS rate constants are in units of hour^{-1}, not day^{-1}, as in PRZM.
Direct photolysis (hour^{-1})	KDP (*,1)	Enter the minimum dark-control corrected environmental aqueous phototransformation rate constant (corresponding to the maximum half-life value). If no aqueous photolysis data are available or if there is no evidence of photolysis, enter zero (0).	Aqueous photolysis data (OPPTS Guideline 835.2240)	Note that this parameter is a rate constant (hour^{-1}), not a half-life (hour). Also note that EXAMS rate constants are in units of hour^{-1}, not day^{-1}, as in PRZM.

Parameter (units)	EXAMS Variable	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Simulated latitude of photolysis test (degrees)	RFLAT	Use the latitude referenced in the aqueous photolysis study.	Aqueous photolysis data (OPPTS Guideline 835.2240)	
Neutral hydrolysis ($hour^{-1}$)	KNH (1,*,1)	Use the minimum hydrolysis rate constant at pH 7 (corresponding to the maximum half-life value). If no hydrolysis data are available, assume that the compound is stable, *i.e.*, enter zero (0).	Hydrolysis data (OPPTS Guideline 835.2120)	Technically, this value represents the neutral hydrolysis rate coefficient. However, if KAH and KBH are set to zero, then the KNH variable represents the overall pH 7 hydrolysis rate. The standard water bodies are set to pH 7. Note that this parameter is a rate constant ($hour^{-1}$), not a half-life (hour). Also note that EXAMS rate constants are in units of $hour^{-1}$, not day^{-1}, as in PRZM.
Partition coefficient for sediment keyed to organic carbon (mL/g_{OC})	KOC (1)	If binding is correlated with organic carbon content, enter the mean K_{OC} and do not enter a K_d value for KPS.	Adsorption/ desorption data (OPPTS Guideline 835.1230)	Binding is correlated with organic carbon content if the coefficient of variation (*i.e.*, the standard deviation divided by the mean) for K_{OC} values is less than that for K_d values. Note that EXAMS calculates a partition coefficient in sediment using the KOC input if the KPS input is not used. The KOW input may be used if both KOC and KPS inputs are not used.

Parameter (units)	EXAMS Variable	Input Value [*Specific Parameter Guidance*]	Data Source	Notes
Partition coefficient for sediment (mL/g)	KPS (*,*)	If binding is not correlated with organic carbon content, enter the mean K_d.	Adsorption/ desorption data (OPPTS Guideline 835.1230)	Binding is correlated with organic carbon content if the coefficient of variation (*i.e.*, the standard deviation divided by the mean) for K_{OC} values is less than that for K_d values.
Molecular weight (g/mole)	MWT (1)	Enter the value for the modeled pesticide.	Calculated	
Aqueous solubility (mg/L)	SOL (*,*)	Enter the maximum value from product chemistry data for the temperature closest to that of the modeled water body.	Product chemistry data	
Vapor pressure (Torr)	VAPR (1)	Enter the maximum value from product chemistry data for the temperature of the modeled water body.	Product chemistry data	
Sediment bacteria temperature coefficient (decimal)	QTBAS (*,*,1)	Enter 2.	Standard value	
Water bacteria temperature coefficient (decimal)	QTBAW (*,*,1)	Enter 2.	Standard value	

Appendix A. Calculating the 90th percentile confidence bound on the mean half-life value.

- If more than one half-life value is available, use Equation 1 to calculate the 90th percentile confidence bound on the mean half-life value:

$$t_{input} = \overline{t_{1/2}} + \frac{t_{90,n-1}s}{\sqrt{n}} \qquad \text{Equation 1}$$

where,

t_{input} = half-life input value (*time*)

$\overline{t_{1/2}}$ = mean of sample half-lives (*time*)

s = sample standard deviation (*time*)

n = number of half-lives available (-)

$t_{90,n-1}$ = one-sided Student's t value at $\alpha = 0.1$ (*i.e.*, 1.0-0.9) (-)

This equation does not calculate the 90th percentile of the distribution of half-life values.

Some Student's t values include:

n-1	1	2	3	4	5	6	7	8	9	10	11	12	∞
t_{90}	3.078	1.886	1.638	1.533	1.476	1.440	1.415	1.397	1.383	1.372	1.363	1.356	1.282

- If only one half-life value is available, use Equation 2 instead of Equation 1 to account for uncertainty in the environmental variability:

$$t_{input} = 3 \times t_{1/2} \qquad \text{Equation 2}$$

- If a first-order rate constant is needed, use Equation 3 to convert the half-life input value from Equation 1 or 2 to a rate constant input value:

$$k_{input} = \frac{\ln(2)}{t_{input}} \qquad \text{Equation 3}$$

where,

k_{input} = rate constant input value ($time^{-1}$)

Appendix B. Update History for the Input Parameter Guidance.

October 22, 2009 (Version 2.1): The following updates were implemented.

- Updated parameter descriptions to better resemble how they appear in the models and reformatted tables to place all parameter descriptions in the left column and order them as they occur in the models.
- Moved to an appendix guidance on calculating the upper 90th percentile of the mean, which is referenced by the guidance for many parameters.
- Harmonized across all surface water models the guidance for soil-water partition coefficients, *i.e.*, to use mean K_{OC} when binding is correlated to organic carbon content and to use mean K_d otherwise.
- Added suggested incorporation depths for different application methods.
- Addressed output file-related parameters not addressed in the previous version (*i.e.*, run number, file name, chemical name, crop name).
- Added other clarifications and made editorial corrections.

GENEEC:

- Added guidance for follow-up parameters (*e.g.*, nozzle height, spray quality, *etc.*) after that for the 'method of application' parameter.

PRZM:

- Added the spray drift fraction (0.03) for ecological exposure assessment of air-blast spray.
- Clarified that this guidance is for using PRZM directly rather than through a graphical user interface (GUI) to estimate exposure in runoff.

EXAMS:

- Clarified that when multiple rate constants are available from hydrolysis or aqueous photolysis studies, the minimum value should be used.
- Clarified that the photolysis input value should reflect the environmental dark control-corrected value, not simply the laboratory dark control-corrected value.
- Removed the instruction to multiply aqueous solubility values by 10.
- Added instruction that if K_{OC} is used, the K_d input should be left blank.
- Clarified that this guidance is for using EXAMS directly rather than through a GUI.